

# THE MERCK INDEX

TENTH EDITION

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AN ENCYCLOPEDIA OF  
CHEMICALS, DRUGS, AND BIOLOGICALS

TENTH EDITION

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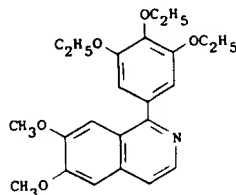
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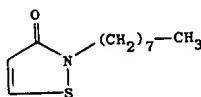
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Asta Chemische Fabrik); cf. Goldberg, Shapero, *J. Pharm. Pharmacol.* 6, 171 (1954).



Free base. Insol in water.  
Hydrochloride,  $C_{23}H_{37}NO_3 \cdot HCl$ , crystals, mp 199-200°. Sparingly sol in water (1:500). Aq solns are acid to litmus.  
THERAP CAT: Antispasmodic.

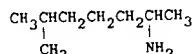
**6597. Oethilnone.** 2-Octyl-3(2H)-isothiazolone; 2-octyl-4-isothiazolin-3-one; RH-893; Kathon.  $C_{11}H_{19}NOS$ ; mol wt 213.34. C 61.93%, H 8.97%, N 6.57%, O 7.50%, S 15.03%. Prepn: S. N. Lewis *et al.*, Fr. pat. 1,555,416 corresp to U.S. pat. 3,761,488 (1969, 1973 to Rohm & Haas); *idem*, *J. Heterocycl. Chem.* 8, 571 (1971).



Liquid, bp<sub>0.01</sub> 120°. uv max (methanol): 280 nm (log  $\epsilon$  3.88).

USE: Fungicide. Biocide in cooling-tower water, paints, cutting oils, cosmetics and shampoo; for leather preservation.

**6598. Octodrine.** 6-Methyl-2-heptanamine; 6-methyl-2-heptylamine; 2-methyl-6-aminoheptane; 6-amino-2-methylheptane; 2-amino-6-methylheptane;  $\alpha,\epsilon$ -dimethylhexylamine; 1,5-dimethylhexylamine; SKF 51; Vaporpac.  $C_8H_{19}N$ ; mol wt 129.24. C 74.34%, H 14.82%, N 10.84%. Prepd from the corresponding saturated ketone: Rohrmann, Shonle, *J. Am. Chem. Soc.* 66, 1516 (1944). Pharmacology: E. J. Fellows, *J. Pharmacol. Exp. Ther.* 90, 351 (1947).

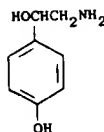


dl-Form, viscous liquid, fishy odor, bp 154-156°.  $n_D^{20}$  1.4200.

Hydrochloride,  $C_8H_{19}N \cdot HCl$ , crystals, sol in water. LD<sub>50</sub> i.p. in mice, rats: 59, 41.5 mg/kg, E. J. Fellows, *loc. cit.*

Sulfate,  $2C_8H_{19}N \cdot H_2SO_4$ , crystals, sol in water.  
THERAP CAT: Adrenergic (vasoconstrictor), local anesthetic.

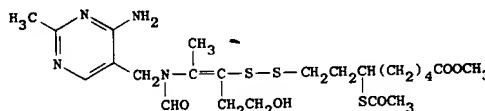
**6599. Octopamine.**  $\alpha$ -(Aminomethyl)-4-hydroxybenzene-methanol;  $\alpha$ -(aminomethyl)-p-hydroxybenzyl alcohol; 1-(p-hydroxyphenyl)-2-aminoethanol; norsympatol; norsynephrine; p-hydroxyphenylethanolamine; WV 569.  $C_9H_{11}NO_2$ ; mol wt 153.18. C 62.72%, H 7.24%, N 9.14%, O 20.89%. Biogenic amine formed by  $\beta$ -hydroxylation of tyramine by the enzyme dopamine  $\beta$ -hydroxylase: Pisano *et al.*, *Biochim. Biophys. Acta* 43, 566 (1960). Identification: Erspamer, *Nature* 169, 375 (1952). Found in the salivary glands of *Octopus vulgaris*, *O. macropus*, and of *Eledone moschata*: *idem*, *Arzneimittel-Forsch.* 2, 253 (1952); in mammalian nerves: Molinoff, Axelrod, *Science* 164, 428 (1969); in cockroach nervous system: Nathanson, Greengard, *ibid.* 180, 308 (1973). Prepd synthetically: Asscher, U.S. pat. 2,585,988 (1952). The natural d(-) form is 3 times more potent than the l(+) form in producing cardiovascular adrenergic responses in anesthetized dogs and cats. Korol, Soffer, *The Pharmacologist* 5, 247 (1963). Prepn of D- and L-forms: Kappe, Armstrong, *J. Med. Chem.* 7, 569 (1964). In invertebrate nervous systems octopamine may function as a neurotransmitter: Saavedra *et al.*, *Science* 185, 364 (1974).



D(-)-Form, crystals from hot water which change at about 160° to a compd which melts at >250° (dec).  $[\alpha]_D^{25}$  -56.0° (0.1 N HCl); -37.4° (H<sub>2</sub>O).  
DL-Form hydrochloride,  $C_8H_{12}ClNO_2$ , *Epiprenor*, *Norden*, *Norfen*, *Norphen* (ampules). Crystals, dec 170°. Freely sol in water.

THERAP CAT: Adrenergic.

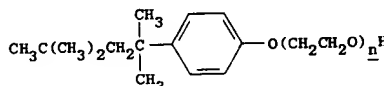
**6600. Octotiamine.** 6-(Acetylthio)-8-[[2-[(4-amino-2-methyl-5-pyrimidinyl)methyl]formylamino]-1-(2-hydroxyethyl)-1-propenyl]dithiooctanoic acid methyl ester; 8-[[2-[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]formamido]-1-(2-hydroxyethyl)propenyl]dithio]-6-mercaptooctanoic acid methyl ester (Stor 6)-acetate; S-(3-acetylthio-7-carbomethoxyheptylthio)thiamine; thiamine 8-(methyl 6-acetyldihydrothioate) disulfide; Gerostop; Neuvitan; TATD.  $C_{32}H_{36}N_4O_6S_3$ ; mol wt 544.87. C 50.72%, H 6.66%, N 10.28%, O 14.68%, S 17.66%. Prepn: Ohara *et al.*, U.S. pat. 3,098,856 (1963 to Fujisawa).



Crystals, mp 106-109°. uv max: 234, 277 nm ( $\epsilon$  16,200, 5820).

Hydrochloride,  $C_{32}H_{36}N_4O_6S_3 \cdot HCl$ , crystals from ether + abs ethanol, mp 134.5-135°. uv max: 233 nm ( $\epsilon$  23,000).  
THERAP CAT: Long-acting oral thiamine.

**6601. Octoxynol.**  $\alpha$ -[4-(1,1,3,3-Tetramethylbutyl)phenyl]- $\omega$ -hydroxypoly(oxy-1,2-ethanediyl); octylphenoxy polyethoxyethanol; polyethylene glycol p-isooctylphenyl ether. Prepd by reacting isooctylphenol with ethylene oxide. Refs. nomenclature, see nonoxynol. Trademarks for series of octoxynols include *Igepal CA*, *Polytergent G*, *Triton X*.



Octoxynol (N.F.), mixture in which  $n$  ranges from 5 to 15; average comp. ( $n = 10$ ):  $C_{34}H_{62}O_{12}$ ; av. mol wt 647. Pale yellow, viscous liquid.  $d_4^{25}$  1.0595.  $n_D^{25}$  1.4894. Miscible with water, alcohol, acetone. Sol in benzene, toluene. Insol in petr ether. pH of 5% aq soln: 7-9. *Octoxynol-9* (USAN), average comp. ( $n = 9$ ):  $C_{32}H_{58}O_{11}$ . Trademarks of products where  $n = 9$  to 10: *Conco NIX-100*, *Igepal CA-630*, *Neutro-nyx 605*, *Triton X-100*. Ingredient of *Preceptin*.

USE: Nonionic detergent, emulsifier, dispersing agent. Ingredient of nitrofurazone soln, N.F.

THERAP CAT: Spermatocide.

**6602. Octyl Acetate.** Acetic acid  $\alpha$ -ethylhexyl ester; 2-ethylhexyl acetate.  $C_{10}H_{20}O_2$ ; mol wt 172.26. C 69.72%, H 11.70%, O 18.58%.  $CH_3(CH_2)_3CH(C_2H_5)CH_2OOCCH_3$ .

Liquid.  $d_4^{20}$  0.873. bp 199°. Solidifies about -80°.  $n_D^{20}$  1.4204. Flash pt, open cup: 190°F (88°C); closed cup: 56°F (13°C). Very slightly sol in water; misc with alcohol, oils, and other organic liquids. LD<sub>50</sub> orally in rats: 3.0 g/kg, H. F. Smyth, C. P. Carpenter, *J. Ind. Hyg. Toxicol.* 26, 269 (1944).

USE: Solvent for nitrocellulose, some resins, waxes, and oils.

**6603. n-Octyl Bromide.** 1-Bromooctane.  $C_8H_{17}Br$ ; mol wt 193.13. C 49.75%, H 8.87%, Br 41.38%.  $CH_3(CH_2)_6CH_2Br$ . Prepd from hydrobromic acid and n-octanol: O.